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A NEW EFFECTIVE-FIELD THEORY FOR THE POTTS MODEL

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ABSTRACT

A new type of effective field theory that has recently been used with success for many applications concerning the Ising model is through the generalization of Callen identities, herein extended to the q-state Potts model. Although mathematically simple, it yields results quite superior to those currently obtained within the Molecular Field Approximation. In order to test its reliability we check the following properties: (a) the critical temperature T_c associated with a linear chain vanishes for all q; (b) the value of T_c associated with a z - coordinated lattice $(z > 2)$ exhibits a q-dependence qualitatively (and to a certain extent quantitatively) satisfactory; (c) the $z \to \infty$ limit reproduces the exact value for T_c; (d) for fixed z, all values of $q > 2$ provide first order phase transitions, which is exact for $d > 4$. Furthermore the procedures for obtaining, as functions of temperature and for any values of q and z, the order parameter, internal energy and specific heat are outlined, and some typical illustrations are presented.

I - INTRODUCTION

Recently Honmura and Kaneyoshi[1] have introduced a new type of effective field treatment of the Ising model. This theory is based on the use of a convenient differential operator into Callen identities[2] and has been applied with success in many different situations such as pure[3-5], site-random[6], bond-random[7,8] Ising bulk properties as well as surface ones[9,10]. Although mathematically simple, this type of approach has proved to be quite superior to the standard Mean Field Approximation (MFA); it leads to vanishing critical temperature T_c for one-dimensional systems, provides a non vanishing "tail" for the specific heat above T_c for higher-dimensional systems and exhibits subtle and physically desirable non uniform convergences associated with various crossovers in random magnetism (see Ref.[8] and references therein).

The q-state Potts model[11] (for an excellent review see Ref. [12]) contains the spin - $\frac{1}{2}$ Ising one as its q=2 particular case; furthermore it is[13], in the limit $q \to 1$, isomorphic to bond percolation. The richness of its thermal properties as well as its numerous applications makes worthy the effort to develop frameworks within which this model can be studied. Herein we extend to the Potts model the effective field approximation we mentioned before. This is done for the pure Potts ferromagnet but, following along Ref.[8], could easily cover also random magnets, including those in which competitive interactions are present. The results will prove, as already mentioned for the Ising case, to be superior to those currently obtained within the MFA (see Refs. [14,15]).

We present in Section II the formalism, including the generalization of Callen's first identity as well as the equation determining, for all q, the order parameter as a function of temperature and external field; in Section III we discuss several important particular cases; finally in Section IV we outline, through the extension of Callen's second identity, the procedure for calculating the internal energy and specific heat as functions of temperature.

II - FORMALISM

II. 1 - Model and generalized Callen first identity

We consider the following Hamiltonian:

$$\mathcal{H} = - q \sum_{i,j} J_{ij} \delta_{\sigma_i,\sigma_j} - q \sum_i h_i \delta_{\sigma_i,0} \tag{1}$$

where $\sigma_i = 0,1,2,\ldots,q-1$, $\forall$ i, $\delta_{\sigma_i,\sigma_j}$ denotes Kronecker's delta function and $h_i \geqslant 0$. The order parameter $m \equiv \langle m_k \rangle \in [0,1]$ associated with this model is determined by

$$m_k \equiv \frac{q\, \delta_{\sigma_k,0} - 1}{q - 1} \tag{2}$$

Let us decompose Hamiltonian (1) into two parts:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}' \tag{3}$$

where

$$\mathcal{H}_0 \equiv - q \sum_j J_{kj} \delta_{\sigma_k,\sigma_j} - q h_k\, \delta_{\sigma_k,0} \tag{4a}$$

and

$$\mathcal{H}' \equiv - q \sum_{i,j}{}' \delta_{\sigma_i,\sigma_j} - q \sum_i{}' h_i \delta_{\sigma_i,0} \tag{4b}$$

where Σ' excludes the k-th site. If we consider now an arbitrary function $f(\sigma_k)$ of the random variable σ_k we obtain:

$$< f(\sigma_k) > \equiv \frac{\underset{\{\sigma_i\}}{\mathrm{Tr}}\, f(\sigma_k)\, e^{-\beta(H_0 + H')}}{\underset{\{\sigma_i\}}{\mathrm{Tr}}\, e^{-\beta(H_0 + H')}}$$

$$= \frac{\underset{\{\sigma_i\}}{\mathrm{Tr}} \left\{ \frac{\underset{\sigma_k}{\mathrm{Tr}}\, f(\sigma_k)\, e^{-\beta H_0}}{\underset{\sigma_k}{\mathrm{Tr}}\, e^{-\beta H_0}} \right\} e^{-\beta H}}{\underset{\{\sigma_i\}}{\mathrm{Tr}}\, e^{-\beta H}}$$

$$\equiv \left\langle \frac{\underset{\sigma_k}{\mathrm{Tr}}\, f(\sigma_k)\, e^{-\beta H_0}}{\underset{\sigma_k}{\mathrm{Tr}}\, e^{-\beta H_0}} \right\rangle$$

$$= \left\langle \frac{\sum_{\sigma_k=0}^{q-1} f(\sigma_k)\, e^{\sum_j K_{k,j}\delta_{\sigma_k,\sigma_j} + L_k \delta_{\sigma_k,0}}}{\sum_{\sigma_k=0}^{q-1} e^{\sum_j K_{k,j}\delta_{\sigma_k,\sigma_j} + L_k \delta_{\sigma_k,0}}} \right\rangle \tag{5}$$

where $\beta \equiv 1/k_B T$, $K_{kj} \equiv \beta q J_{kj}$ and $L_k \equiv \beta q h_k$.

By choosing now $f(\sigma_k) = \delta_{\sigma_k,0}$ into Eq.(5) we obtain

$$\langle\delta_{\sigma_k,0}\rangle = \left\langle \frac{e^{\sum\limits_j K_{k,j}\delta_{0,\sigma_j} + L_k}}{e^{\sum\limits_j K_{k,j}\delta_{0,\sigma_j} + L_k} + \sum\limits_{\sigma_k=1}^{q-1} e^{\sum\limits_j K_{k,j}\delta_{\sigma_k,\sigma_j}}} \right\rangle \tag{6}$$

which generalizes the site Callen identity to all values of q. Notice also that the following sum rule is satisfied:

$$\delta_{0,\sigma_j} + \sum_{\sigma_k=1}^{q-1} \delta_{\sigma_k,\sigma_j} = 1 \ , \ \forall\ \sigma_j \tag{7}$$

hence

$$<\delta_{0,\sigma_j}> + (q-1) < \delta_{1,\sigma_j}> = 1, \ \forall\ \sigma_j \tag{7'}$$

It is straightforward to verify that the use of Eqs.(6) and (7) yields, for q=2, the standard Callen identity

$$< m_k > = < \tanh\beta(\sum_j J_{kj}m_j + h_k) > \tag{8}$$

II.2 - <u>Differential operator and order parameter</u>

By introducing the differential operator $D_n \equiv \partial/\partial X_n$ (n=0,1,2, ..., q-1) we verify

$$e^{\alpha D_r} f(X_0,X_1, \ldots, X_r, \ldots, X_{q-1}) = f(X_0,X_1, \ldots, X_r+\alpha, \ldots, X_{q-1}) \tag{9}$$

where $f(\{X_n\})$ is any analytic function. Consequently Eq.(6) can be rewritten as follows:

$$< \delta_{\sigma_k,0} > = < \prod_{n=0}^{q-1} e^{D_n \sum_j K_{k,j} \delta_{n,\sigma_j}} > \left. \frac{e^{L_k+X_0}}{e^{L_k+X_0} + \sum_{n=1}^{q-1} e^{X_n}} \right|_{\{X_n\}=0} \tag{10}$$

By using now the property

$$e^{D_n K_{k,j} \delta_{n,\sigma_j}} = 1 + (e^{D_n K_{k,j}} - 1)\delta_{n,\sigma_j} \tag{11}$$

as well as the sum rule given by Eq.(7a) we can finally rewrite Eq.(10) as follows:

$$< \delta_{\sigma_k,0} > = < \prod_j \sum_{n=0}^{q-1} e^{D_n K_{k,j}} \delta_{n,\sigma_j} > \left. \frac{e^{L_k+X_0}}{e^{L_k+X_0} + \sum_{n=1}^{q-1} e^{X_n}} \right|_{\{X_n\}=0} \tag{12}$$

Up to this point there has been no approximation and Eq.(12) is exact; unfortunately its further development seems untractable and consequently we shall introduce an approximate decoupling (see [8] and references therein for the q=2 case) and rewrite Eq.(12) as follows:

$$< \delta_{\sigma_k,0} > = \prod_j < \sum_{n=0}^{q-1} e^{D_n K_{k,j}} \delta_{n,\sigma_j} > \left. \frac{e^{L_k+X_0}}{e^{L_k+X_0} + \sum_{n=1}^{q-1} e^{X_n}} \right|_{\{X_n\}=0} \tag{13}$$

Let us from now on consider first-neighbour interactions (with coupling constant $K_{k,j} \equiv K$) in a z-coordinated regular lattice (z=2d for the d-dimensional hypercubic lattices); Eq.(13) becomes

$$< \delta_{\sigma_k,0} > = \left\langle \sum_{n=0}^{q-1} e^{D_n K} \delta_{n,\sigma_j} \right\rangle^z \left. \frac{e^{L_k+X_0}}{e^{L_k+X_0} + \sum_{n=1}^{q-1} e^{X_n}} \right|_{\{X_n\}=0}$$

$$= \left\{ e^{D_0 K} < \delta_{\sigma_j,0} > + \frac{1 - < \delta_{\sigma_j,0} >}{q-1} \sum_{n=1}^{q-1} e^{D_n K} \right\}^z \left. \frac{e^{L_k+X_0}}{e^{L_k+X_0} + \sum_{n=1}^{q-1} e^{X_n}} \right|_{\{X_n\}=0} \tag{14}$$

By using Eq.(2) we obtain the equation of states:

$$1 + (q-1)m = \frac{1}{q^{z-1}} \left\{ e^{D_0 K} [1+(q-1)m] + (1-m) \sum_{n=1}^{q-1} e^{D_n K} \right\}^z \left. \frac{e^{L_k+X_0}}{e^{L_k+X_0} + \sum_{n=1}^{q-1} e^{X_n}} \right|_{\{X_n\}=0} \tag{15}$$

And finally by developing, through the Leibnitz formula, the z-power and performing the differential operations we obtain, for $L_k=0$, the equation of states:

$$1 + (q-1)m = \frac{1}{q^{z-1}} \sum_{\{n_i\}} \frac{z!}{n_0!\, n_1! \ldots n_{q-1}!} [1+(q-1)m]^{n_0} (1-m)^{z-n_0} \frac{e^{n_0 K}}{\sum_{i=0}^{q-1} e^{n_i K}} \tag{16}$$

where the sum runs over all the partitions $\{n_i\}$ satisfying the condition

$$\sum_{i=0}^{q-1} n_i = z \tag{17}$$

In the neighborhood of the critical temperature T_c (i.e. $m \to 0$) Eq.(16) provides

$$m \sim Am + Bm^2 \tag{18}$$

where we have used the fact that, for all K,

$$\sum_{\{n_i\}} \frac{z!}{n_0! n_1! \ldots n_{q-1}!} \frac{e^{n_0 K}}{\sum_{i=0}^{q-1} e^{n_i K}} = q^{z-1} , \tag{19}$$

$$A \equiv \frac{1}{(q-1)q^{z-1}} \sum_{\{n_i\}} \frac{z!}{n_0!\, n_1! \ldots n_{q-1}!} (qn_0 - z) \frac{e^{n_0 K}}{\sum_{i=0}^{q-1} e^{n_i K}} \tag{20}$$

and where

$$B \equiv \frac{1}{(q-1)q^{z-1}} \sum_{\{n_i\}} \frac{z!}{n_0!\, n_1! \ldots n_{q-1}!} \times$$

$$\left[\frac{n_0(n_0-1)(q-1)^2 + (z-n_0)(z-n_0-1)}{2} - n_0(z-n_0)(q-1)\right] \frac{e^{n_0 K}}{\sum_{i=0}^{q-1} e^{n_i K}} \tag{21}$$

The critical temperature T_c associated with a second order phase transition satisfies

$$A(T_c) = 1 \tag{22}$$

Typical values of T_c are presented in Fig.1. We can verify that if $B(T_c) < 0$ the transition is a second order one and m vanishes linearly with T ($dm/dT|_{T_c} < 0$);if B=0 the transition still is a second order one and m vanishes not less abruptly than $(T_c-T)^{1/2}$; if $B > 0$ the phase transition is a first order one and the transition occurs in fact at a temperature $T_0 > T_c$. We verify also that B=0 for q=2 and all values of $z \geqslant 2$ (z=2 corresponds to a linear chain).

III - PARTICULAR CASES

III.1 - Ising model (q=2)

For q=2 and all values of z the critical temperature T_c satisfies

$$\frac{1}{2^{z-1}}\left\{\sum_{i=0}^{[2z-3-(-1)^z]/4} \frac{z!(z-2i)}{i!(z-i)!} \tanh \frac{z-2i}{t}\right\} = 1 \tag{23}$$

where we have used Eqs.(20) and (22) and

$$t \equiv \frac{2}{K} = \frac{k_B T}{J} \tag{24}$$

For z=2,3,4 and 6 we recover previous results[7,8]; Eq.(23) is a simplified form of Eq.(22) of Ref.[7].

From Eq.(16) we obtain the full equation of states, which is given by

$$m = \frac{1}{2^z}\left\{\sum_{i=0}^{[2z-3-(-1)^z]/4} \frac{z!}{i!(z-i)!} \times \right.$$

$$\left. [(1-m)^i(1+m)^{z-i} - (1+m)^i(1-m)^{z-i}] \tanh \frac{z-2i}{t}\right\} \tag{25}$$

This expression recovers, for z=2,3,4 and 6, previous results[7,8]; it admits, for all values of $z > 2$, the trivial solution $m \equiv 0$ (paramagnetic phase) and a non trivial one for $T < T_c$ (ferromagnetic phase), the transition being a second order one.

III.2 - Linear Chain (z=2)

For z=2 and all values of q, Eq.(16) yields

$$m = Am + Bm^2 \tag{26}$$

with

$$A \equiv \frac{2}{q}\left[\frac{e^{2K} - 1}{e^{2K} + (q-1)} + \frac{(q-2)(e^{K}-1)}{2e^{K} + (q-2)} \right] \tag{27}$$

and

$$B \equiv (q-2) \frac{(e^{K} - 1)^2}{[e^{2K}+(q-1)]\,[2e^{K}+(q-2)]} \tag{28}$$

The analysis of Eq.(26) shows that, for $q \geqslant 2$, m vanishes at any finite temperature, therefore $T_c=0$, which is the exact result (not reproducible within the MFA). For $q < 2$, both $m \equiv 0$ and $m \neq 0$ solutions exist, however the discussion of the free energy should show that $m \neq 0$ is an unstable solution.

III.3 - Infinite-range forces ($z \to \infty$)

We consider herein that each spin interacts with a bigger and bigger number z of other spins, through a reduce exchange K which is smaller and smaller in such a way that Kz remains finite (this ensures the extensivity of quantities such as the free and internal energies). We go back to Eq. (15) with $L_k=0$, and consider the operator which appears therein:

$$\left\{ \frac{1}{q}[1+(q-1)m]e^{D_0 K} + \frac{1-m}{q} \sum_{n=1}^{q-1} e^{D_n K} \right\}^z$$

$$= \exp\left\{ z \ln \left\{ \frac{1}{q}[1+(q-1)m]e^{D_0 K} + \frac{1-m}{q} \sum_{n=1}^{q-1} e^{D_n K} \right\}\right\}$$

$$\sim \exp\left\{ z \ln \left[1+ \frac{1+(q-1)m}{q} KD_0 + \frac{1-m}{q} K \sum_{n=1}^{q-1} D_n\right] \right\}$$

$$\sim \exp\left\{ z \left[\frac{1+(q-1)m}{q} KD_0 + \frac{1-m}{q} K \sum_{n=1}^{q-1} D_n\right] \right\} \tag{29}$$

By replacing this operator into Eq.(15) we obtain

$$1 + (q-1)m \sim \frac{q\, e^{\frac{zK}{q}[1+(q-1)m]}}{e^{\frac{zK}{q}[1+(q-1)m]} + (q-1)\, e^{\frac{zK}{q}(1-m)}} \tag{30}$$

hence

$$e^{-zKm} \sim \frac{1-m}{1+(q-1)m} \tag{31}$$

This equation is precisely that obtained in Ref.[14] within a MFA framework, i.e. the present approach is equivalent to a MFA for all values of q and $z \to \infty$. Eq.(31) provides, for $q < 2$ ($q > 2$), a second (first) order phase transition occuring at $K_c^{-1} \simeq z/q$ ($K_c^{-1} > z/q$); see Fig.2. These results are known[12] to be exact.

III.4 - Typical cases ($z > 2$; $q > 2$)

In order to present typical curves we extract from Eq.(16) a few cases, namely ($q = 3$; $z = 4,6$) and ($q = 4$; $z = 4$).

For $q = 3$ and $z = 4$ we obtain:

$$m = Am + Bm^2 + Cm^3 + Dm^4 \tag{32}$$

where

$$A \equiv 11-4\left[\frac{2}{e^{4K}+2} + \frac{4e^K+6}{e^{3K}+e^K+1} + \frac{3}{2e^{2K}+1} + \frac{6}{e^K+2}\right] \tag{33}$$

$$B \equiv 6-6\left[\frac{2}{e^{4K}+2} + \frac{4e^K}{e^{3K}+e^K+1} - \frac{3}{2e^{2K}+1}\right] \tag{34}$$

$$C \equiv -24-24\left[\frac{1}{e^{4K}+2} - \frac{e^K}{e^{3K}+e^K+1} - \frac{3}{e^K+2}\right] \tag{35}$$

$$D \equiv 8-2\left[\frac{5}{e^{2K}+2} - \frac{8e^K+12}{e^{3K}+e^K+1} + \frac{3}{2e^{2K}+1} + \frac{24}{e^K+2}\right] \tag{36}$$

For $q = 4$ and $z = 4$ we obtain once more Eq.(32) where

$$A \equiv 3 - \left[\frac{1}{e^{4K}+3} + \frac{2e^{K}+6}{e^{3K}+ e^{K}+2} + \frac{6e^{K}+6}{e^{2K}+ 2e^{K}+1} + \frac{3}{2e^{2K}+2} \right] \tag{37}$$

$$B \equiv 3-3 \left[\frac{1}{e^{4K}+3} + \frac{2e^{K}+2}{e^{3K}+ e^{K}+2} + \frac{2e^{K}-2}{e^{2K}+2\ e^{K}+1} - \frac{1}{2e^{2K}+2} \right] \tag{38}$$

$$C \equiv -8- \left[\frac{7}{e^{4K}+3} - \frac{2e^{K}-2}{e^{3K}+ e^{K}+2} - \frac{30e^{K}+6}{e^{2K}+ 2e^{K}+1} - \frac{3}{2e^{2K}+2} \right] \tag{39}$$

$$D \equiv 3 - \left[\frac{5}{e^{4K}+3} - \frac{6e^{K}+14}{e^{3K}+ e^{K}+2} + \frac{18e^{K}+6}{e^{2K}+ 2e^{K}+1} + \frac{3}{2e^{2K}+2} \right] \tag{40}$$

For q = 3 and z = 6 we obtain:

$$m = Am + Bm^{2} + Cm^{3} + Dm^{4} + Em^{5} + Fm^{6} \tag{41}$$

where

$$A \equiv 487 - 6 \left[\frac{2e^{6K}-2}{e^{6K}+2} + \frac{18e^{5K}-6\ e^{K}-12}{e^{5K}+ e^{K}+1} + \frac{30e^{4K}-30}{e^{4K}+ e^{2K}+1} \right.$$

$$\left. + \frac{30e^{4K}-30\ e^{K}}{e^{4K}+ e^{K}} + \frac{20e^{3K}-20}{2e^{3K}+1} + \frac{60e^{3K}-60\ e^{K}}{e^{3K}+ e^{2K}+ e^{K}} \right] \tag{42}$$

$$B \equiv 180-15\left[\frac{4e^{6K}+2}{e^{6K}+2}+\frac{24e^{5K}+12}{e^{5K}+e^{K}+1}+\frac{18e^{4K}-12e^{2K}+30}{e^{4K}+e^{2K}+1}\right.$$

$$\left.+\frac{18e^{4K}}{e^{4K}+2e^{K}}-\frac{8e^{3K}-20}{2e^{3K}+1}-\frac{24e^{3K}+48e^{2K}}{e^{3K}+e^{2K}+e^{K}}\right] \quad (43)$$

$$C \equiv -120-20\left[\frac{8e^{6K}-2}{e^{6K}+2}+\frac{24e^{5K}+6e^{K}-12}{e^{5K}+e^{K}+1}-\frac{12e^{4K}-6e^{2K}+30}{e^{4K}+e^{2K}+1}\right.$$

$$\left.-\frac{12e^{4K}-30e^{K}}{e^{4K}+2e^{K}}-\frac{22e^{3K}+20}{2e^{3K}+1}-\frac{66e^{3K}-24e^{2K}-60e^{K}}{e^{3K}+e^{2k}+e^{K}}\right] \quad (44)$$

$$D \equiv 270-15\left[\frac{16e^{6K}+2}{e^{6K}+2}-\frac{12e^{K}-12}{e^{5K}+e^{K}+1}-\frac{48e^{4K}-18e^{2K}-30}{e^{4K}+e^{2K}+1}\right.$$

$$\left.-\frac{48e^{4K}+60e^{K}}{e^{4K}+2e^{K}}+\frac{16e^{3K}+20}{2e^{3K}+1}+\frac{48e^{3K}+72e^{2K}-120e^{K}}{e^{3K}+e^{2K}+e^{K}}\right] \quad (45)$$

$$E \equiv 360-6\left[\frac{32e^{6K}-2}{e^{6K}+2}-\frac{96e^{5K}-18e^{K}+12}{e^{5K}+e^{K}+1}-\frac{60e^{2K}+30}{e^{4K}+e^{2K}+1}\right.$$

$$\left.+\frac{90e^{K}}{e^{4K}+2e^{K}}+\frac{80e^{3K}-20}{2e^{3K}+1}+\frac{240e^{3K}-240e^{2K}+180e^{K}}{e^{3K}+e^{2K}+e^{K}}\right] \quad (46)$$

$$F \equiv -120 - \left[\frac{64e^{6K}+2}{e^{6K}+2} - \frac{384e^{5K}+24e^{K}-12}{e^{5K}+e^{K}+1} + \frac{480e^{4K}+120e^{2K}+30}{e^{4K}+e^{2K}+1} \right. \tag{47}$$

$$\left. + \frac{480e^{4K}-120e^{K}}{e^{4K}+2e^{K}} - \frac{320e^{3K}-20}{2e^{3K}+1} - \frac{960e^{3K}-480e^{2K}+240e^{K}}{e^{3K}+e^{2K}+e^{K}} \right] \tag{47}$$

We notice that all three cases (see Eqs. (32) and (41)) admit the paramagnetic $m\equiv 0$ solution as well as the non trivial ferromagnetic one; we present in Fig.3 the curves corresponding to $q=3,4$ and $z=4$, together with those associated with ($q=2$; $z=4,6$) for comparison.

Let us finally remark that the present theory, as the MFA[14], yields, for all values of z (i.e. for all dimensionalities d), first (second) order phase transitions for $q > 2$ ($q \leqslant 2$); this is correct for $d \geqslant 4$ but wrong for $d < 4$ (see for example Ref.[12]).

IV - INTERNAL ENERGY AND SPECIFIC HEAT

IV.1 - Generalized Callen second identity

Let us consider an arbitrary two-site function $f(\sigma_k, \sigma_\ell)$ and use Hamiltonian $\mathcal{H}$ into canonical thermal averages:

$$\langle f(\sigma_k,\sigma_\ell)\rangle \equiv \frac{\mathrm{Tr}\, f(\sigma_k,\sigma_\ell)\, e^{-\beta\mathcal{H}}}{\mathrm{Tr}\, e^{-\beta\mathcal{H}}}$$

$$= \frac{\displaystyle \mathop{\mathrm{Tr}}_{\{\sigma_i\}\neq\sigma_\ell} \sum_{n=0}^{q-1} f(\sigma_k,n)\, e^{L_\ell \delta_{n,0} + \sum_j K_{j\ell}\delta_{\sigma_j,n}}\, e^{-\beta H'}}{\displaystyle \mathop{\mathrm{Tr}}_{\{\sigma_i\}\neq\sigma_\ell} \sum_{n=0}^{q-1} e^{L_\ell \delta_{n,0} + \sum_j K_{j\ell}\delta_{\sigma_j,n}}\, e^{-\beta H'}}$$

$$= \frac{\displaystyle \mathrm{Tr} \sum_{n=0}^{q-1} f(\sigma_{k,n})\, e^{L_\ell \delta_{n,0} + \sum_j K_{j\ell}\delta_{\sigma_j,n}}\, e^{-\beta H}}{\displaystyle \mathrm{Tr} \sum_{n=0}^{q-1} e^{L_\ell \delta_{n,0} + \sum_j K_{j\ell}\delta_{\sigma_j,n}}\, e^{-\beta H}}$$

$$\equiv \left\langle \frac{\displaystyle \sum_{n=0}^{q-1} f(\sigma_k,n)\, e^{L_\ell \delta_{n,0} + \sum_j K_{j\ell}\delta_{\sigma_j,n}}}{\displaystyle \sum_{n=0}^{q-1} e^{L_\ell \delta_{n,0} + \sum_j K_{j\ell}\delta_{\sigma_j,n}}} \right\rangle \tag{48}$$

This expression extends to all values of q the Callen second identity for the Ising model.

IV.2 - Internal energy and specific heat

We consider from now on $L_\ell=0$. By making use of Eq.(48) we may write

$$\left\langle \sum_k K_{k\ell}\delta_{\sigma_k,\sigma_\ell} \right\rangle = \left\langle \frac{\displaystyle \sum_{n=0}^{q-1} \sum_k K_{k\ell}\delta_{\sigma_k,n}\, e^{\sum_j K_{j\ell}\delta_{\sigma_j,n}}}{\displaystyle \sum_{n=0}^{q-1} e^{\sum_j K_{j\ell}\delta_{\sigma_j,n}}} \right\rangle$$

$$= \left\langle \prod_{n=0}^{q-1} e^{D_n \sum_j K_{j\ell} \delta_{\sigma_j, n}} \right\rangle \left. \frac{\sum_{n=0}^{q-1} X_n e^{X_n}}{\sum_{n=0}^{q-1} e^{X_n}} \right|_{\{X_n\}=0} \qquad (49)$$

where we have introduced, in the last step, the differential operators $\{D_n\}$. By using Eqs.(7) and (11), this identity can be rewritten as follows:

$$\left\langle \sum_k K_{k\ell} \delta_{\sigma_k, \sigma_\ell} \right\rangle = \left\langle \prod_j \sum_{n=0}^{q-1} e^{D_n K_{j\ell} \delta_{\sigma_j, n}} \right\rangle \frac{\sum_{n=0}^{q-1} X_n e^{X_n}}{\sum_{n=0}^{q-1} e^{X_n}} \qquad (50)$$

By decoupling as before (i.e. $< \prod_j \ldots > \simeq \prod_j < \ldots >$) and using Eqs. (2) and (7') we obtain

$$\left\langle \sum_k K_{k\ell} \delta_{\sigma_k, \sigma_\ell} \right\rangle = \prod_j \left[\frac{1+(q-1)m}{q} e^{D_0 K_{j\ell}} + \frac{1-m}{q} \sum_{n=1}^{q-1} e^{D_n K_{j\ell}} \right] \times$$

$$\left. \frac{\sum_{n=0}^{q-1} X_n e^{X_n}}{\sum_{n=0}^{q-1} e^{X_n}} \right|_{\{X_n\}=0} \qquad (51)$$

By assuming first-neighbor interactions ($K_{j\ell} \equiv K$) in a z-coordinated regular lattice of N sites and taking into account Hamiltonian (1) (with $h_i=0$ and where each couple (i,j) is counted only once), we can write the internal energy $E \equiv \langle \mathcal{H} \rangle$ as follows:

$$\frac{E}{N} = -\frac{k_B T}{2} \left[\frac{1+(q-1)m}{q} e^{D_0 K} + \frac{1-m}{q} \sum_{n=1}^{q-1} e^{D_n K} \right]^z \left. \frac{\sum_{n=0}^{q-1} X_n e^{X_n}}{\sum_{n=0}^{q-1} e^{X_n}} \right|_{\{X_n\}=0} \qquad (52)$$

By performing the same steps we followed in order to establish Eq.(16) from Eq.(15), we finally obtain:

$$\frac{E}{N} = -\frac{k_B T}{2q^z} \sum_{\{n_i\}} \frac{z!}{n_0!\, n_1! \ldots n_{q-1}!} [1+(q-1)m]^{n_0} (1-m)^{z-n_0} \times \frac{\sum_{i=0}^{q-1} n_i K e^{n_i K}}{\sum_{i=0}^{q-1} e^{n_i K}} \qquad (53)$$

where condition (17) is satisfied. Eq.(53) gives E as a function of $q, z, k_BT/J$ and $m(q,z,k_BT/J)$; consequently it also determines the specific heat $C \equiv dE/dT$ in both para- and ferro-magnetic phases. The type of results that Eq.(53) provides for q=2 and z > 2 can be seen in Ref.[16] (where the diluted Ising model has been discussed); the type of results that it provides for q > 2 and z > 2 are depicted in Fig 4.

V - CONCLUSION

In the present paper the single-site and two-site identities originally established by Callen for the Ising model have been extended to any q-state Potts model. By making use of them and taking advantage of convenient differential operators, an effective field theory is developed, within which the order parameter, internal energy and specific heat can be calculated for all temperatures (the calculation of the susceptibility is also feasible; it is however out of the scope of the present work). This theory, without introducing mathematical complexities, provides results which are quite superior to those obtained within the standard Mean Field Approximation (MFA): a) it provides $T_c = 0$ for the linear chain; b) a "tail" in the paramagnetic specific heat is observed; c) the q- and z- dependences of T_c are satisfactory and numerically closer to the exact (or almost exact) ones than the values provided by MFA. It shares with MFA the classical values for the critical exponents, the fact that the transition is obtained to be of the first (second) order for $q > 2$ ($q \leq 2$), which is correct for $d \geq 4$, as well as the equation of states for $z \to \infty$ and any value of q. The present type of theory has had some success in the discussion of complex Ising systems; the same is expected for analogous Potts models.

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REFERENCES

1- R.Honmura and T.Kaneyoshi, Prog. Theor. Phys. 60, 635 (1978); J.Phys. C 12, 3979 (1979).

2- H.B.Callen, Phys.Lett. 4, 161 (1963).

3- T.Kaneyoshi, I.P.Fittipaldi, R.Honmura and T.Manabe, Phys.Rev. B 24, 481 (1981).

4- G.B.Taggart and I.P.Fittipaldi, Phys. Rev. B 25, 7026 (1982).

5- F.C.Sá Barreto and I.P.Fittipaldi, Ferroelectrics 39, 1103 (1981).

6- R. Honmura, A.F.Khater, I.P.Fittipaldi and T.Kaneyoshi, Solid St. Commun. 41, 385 (1982).

7- T.Kaneyoshi, I.P.Fittipaldi and H.Beyer, Phys. Stat. Solidi B 102, 393 (1980).

8- E.F.Sarmento and C.Tsallis, Phys. Rev. B 27, (1983).

9- T.Kaneyoshi and H.Beyer, J.Phys. Soc. Jpn. 49, 1306 (1980).

10- K.Sakata, E.F.Sarmento, I.P.Fittipaldi and T.Kaneyoshi, Solid Stat Commun. 42, 13 (1982).

11- R.B.Potts, Proc.Camb.Phil.Soc. 48, 106 (1952).

12- F.Y.Wu, Rev.Mod.Phys. 54, 235 (1982).

13- P.W.Kasteleyn and C.M.Fortuin, J.Phys. Soc.Jpn. 26 (Suppl.) 11 (1969).

14- T.Kihara, Y.Midzuno and J.Shizume, J.Phys.Soc. Jpn. 9, 681 (1954).

15- L.Mittag and M.J.Stephen, J.Phys. A 7 , L109 (1974).

16- R.Honmura, E.F.Sarmento and C.Tsallis, Z.fur Physik B (under press; 1983).

CAPTION FOR FIGURES

Fig. 1 - Critical temperatures $T_c(z,q)$ for the q-state Potts ferromagnet in a z-coordinated lattice (the dashed lines are possible analytic extensions for arbitrary z). $k_B T_c(4,2)/J$ equals 3.0892 to be compared with the MFA result 4 and with the exact one 2.27...

Fig. 2 - Thermal dependence of the reduced spontaneous magnetization associated with the $z\to\infty$ q-state Potts ferromagnet.

Fig. 3 - Themal dependence of the reduced spontaneous magnetization associated with typical values of (z,q). The dashed lines are to stress the fact that the transitions herein provided for q>2 are first order ones (hence m is discontinuous).

Fig. 4 - Typical thermal dependences of the specific heat C and internal energy E corresponding to q>2. T_o (T_c) is the critical (disordered phase metastability limit) temperature. The dashed line indicates the thermodynamically unfavorable analytical extension of the curve.

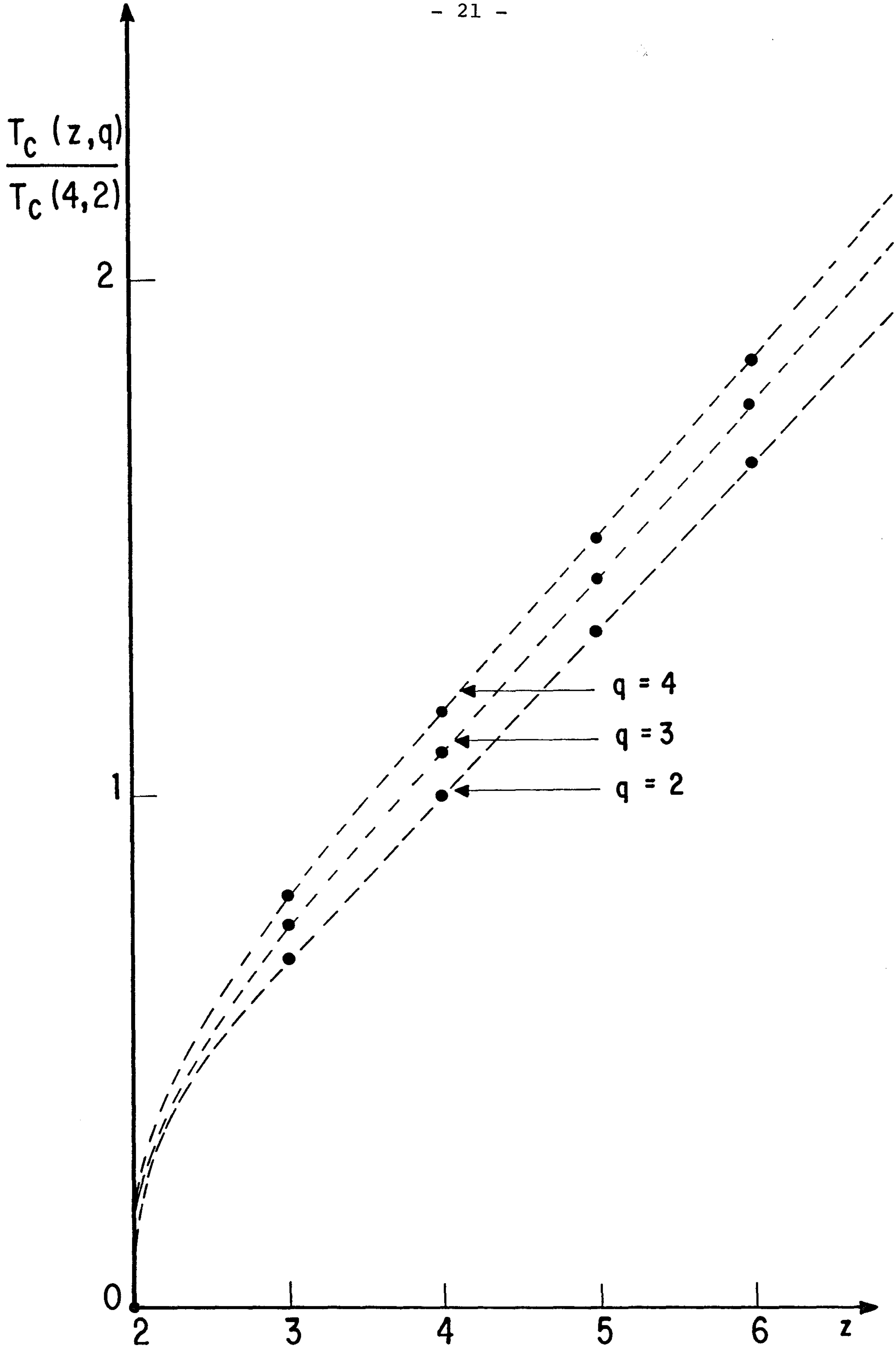

FIG.1

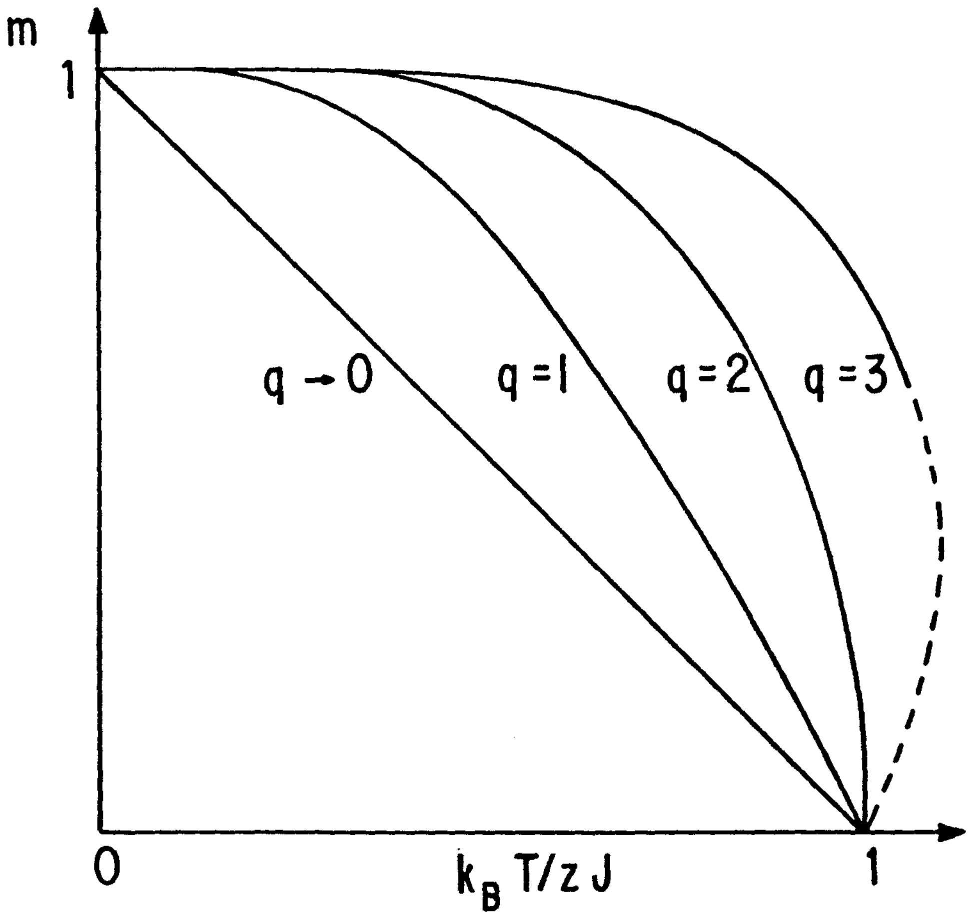

FIG. 2

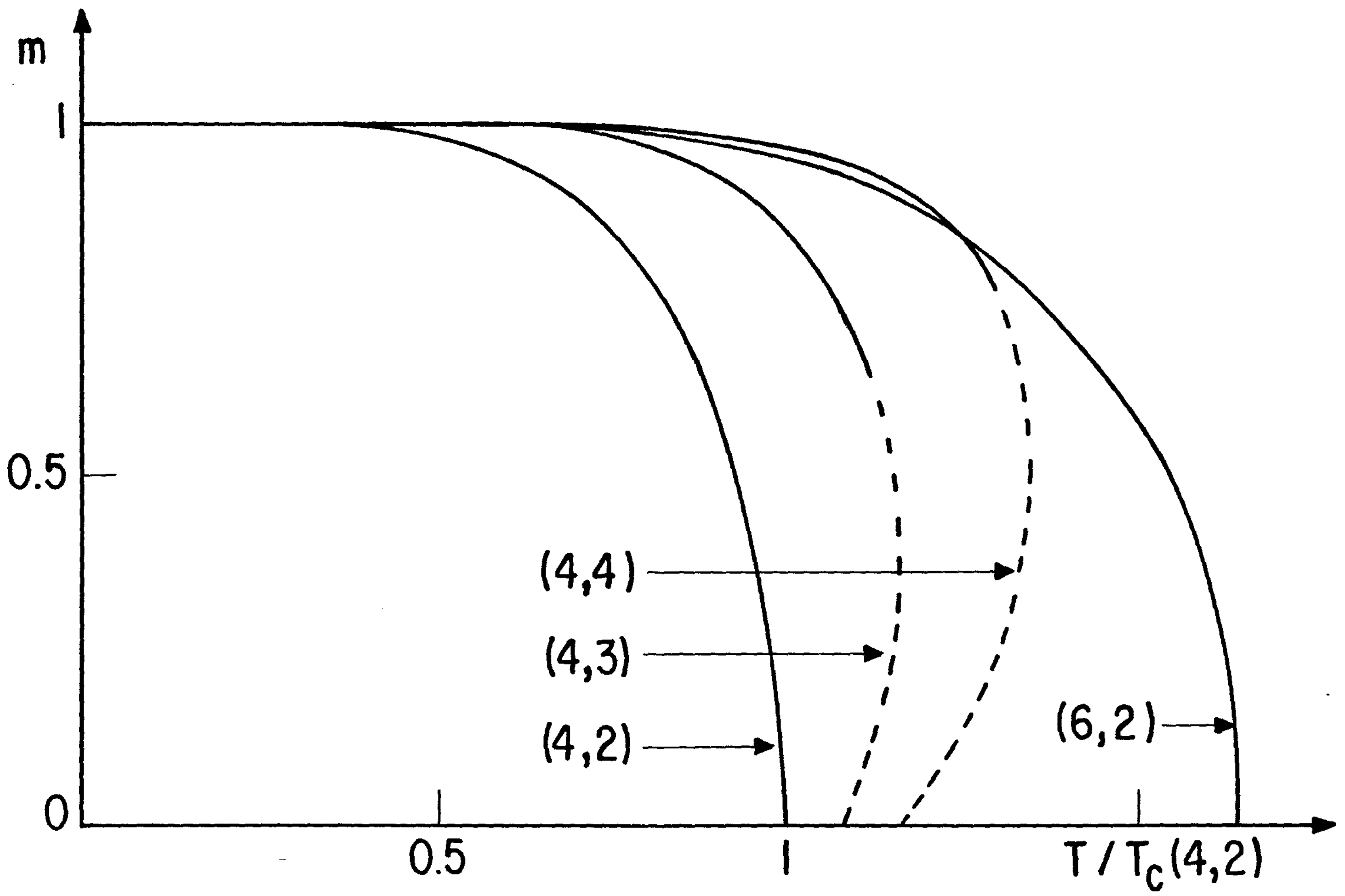

FIG.3

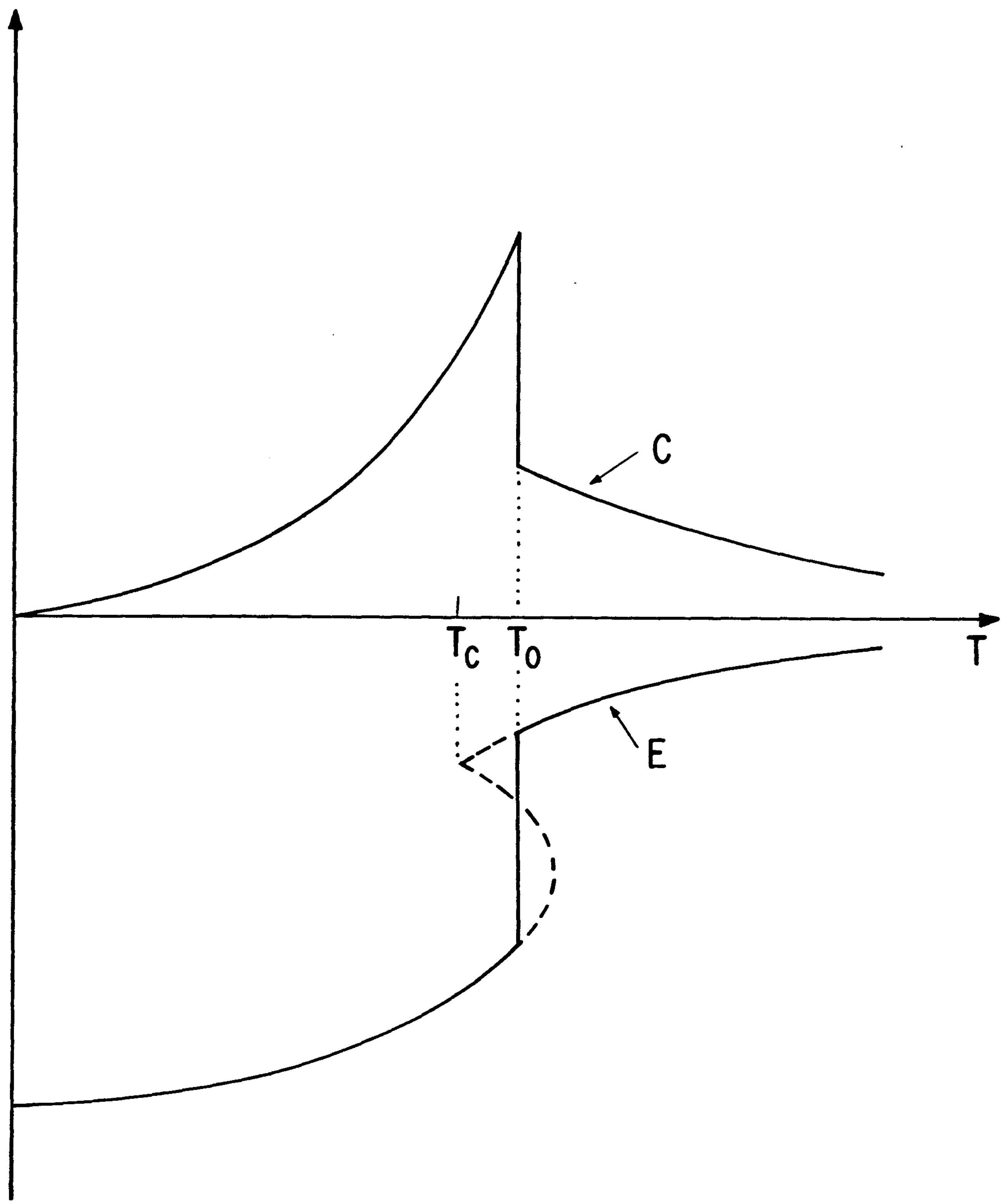

FIG. 4